THE IMPORTANCE OF CHOOSING THE INTERACTION POTENTIAL FOR MD SIMULATIONS IN SOLID CARBON EXTRACTION

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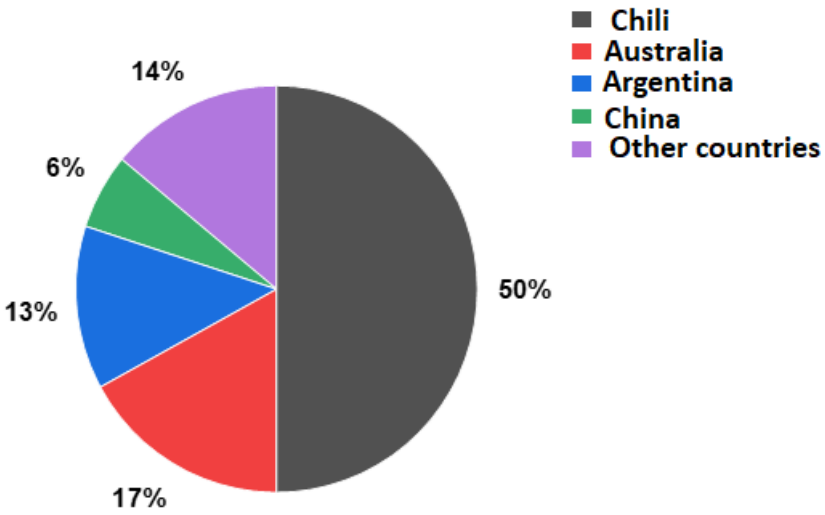
Abstract: Hard carbons are prime candidates for anodes for next-generation sodium-ion batteries for large-scale energy storage. Hard carbons have a more disordered structure, more defects, higher concentration of heteroatoms, larger spacing between graphite layers, and more closed pore structures than soft carbons, which provide more storage sites and diffusion pathways for Na+ ions. In the formation of hard carbons, it is important to correctly select the interaction potential between C-C atoms by molecular dynamics (MD).

Keywords: lithium and sodium-ion batteries, anode, Molecular dynamics (Md), Reaxff, solid carbon, thermostat, Lammps.

Introduction: Technology is developing rapidly around the world, making many of humanity's tasks easier, including smartphones, video cameras, cars, and similar technologies, and many of them are powered by batteries. The use of batteries in technology has increased the demand for them and the production volume has increased dramatically. Lithium-ion batteries (LIB), which are one of the best in the battery market, are not widely distributed and are expensive to produce, so it is becoming more and more urgent to produce a battery with good characteristics through other alternative materials. Sodium-Ion batteries are widely distributed on earth and can compete with LIBs in many aspects.

Lithium-ion batteries (LIBs) are widely used to power electric vehicles, including modern cars such as the Tesla Model S™. Their speed and acceleration performance are competitive with gasoline cars [1]. In 2018, 70% of LIB production was used in the automotive industry, compared to 43% in 2015 and only 6% in 2010. According to forecasts, by 2025, the demand for electric vehicles could lead to the depletion of more than 25% of lithium deposits [2]. Today, lithium reserves are estimated at 15 to 30 million tons. These reserves are mainly located in Chile, Australia, Argentina, and China. However, the recycling rate of lithium from used batteries is only 1%, which further increases the risk of resource shortages [3]. The rapid growth of demand for LIBs for electric vehicles has led to a decrease in lithium resources and an increase in overall costs, making them

economically uneconomical for large-scale energy storage systems. The current world lithium resources and production volume are presented in Figure 1 [4]. As a result, attention is being paid to alternative energy storage systems with large reserves and lower costs, where energy density is not a major issue. In this context, sodium-ion batteries (NIBs) have attracted the attention of researchers, and although they have difficulties competing with LIBs in terms of energy density, they have a number of advantages. The main advantages of NIBs include the fact that sodium is the fourth most abundant element in the earth's crust and their low cost. Because their cathode and electrolyte are made of economical Na-based



compounds. Although LIBs currently have an advantage over many batteries, the limited availability and high cost of lithium require research into other alternative batteries. Researchers are considering NIBs as the best alternative in this regard.

Figure 1. Lithium reserves worldwide (16,000 thousand metric tons)

Method and result: In this study, the molecular dynamics (MD) method of computer modeling of solid carbon, which is the anode material of sodium-ion batteries, was performed using the LAMMPS programming package. The Reaxff effect potential was used to correctly describe the bonding between C-C atoms. In order to generate the process, a simulation box with sides of 24 Å along the x, y, and z axes was randomly filled with carbon atoms. The process consisted of four stages. In stage I, the simulation was brought to thermodynamic equilibrium at a temperature of 300 K in the NVT ensemble using a Nosé-Hoover thermostat for 10 ps, during which the initial velocities were distributed and the temperature of the system was equilibrated. In stage II, the simulation was increased from 300 K to 4500 K in the NVT ensemble using an Andersen barostat over a time interval of 10 ps. In stage III, the temperature was held at 4500 K in the NVT ensemble for a time interval of 1000 ps. In stage IV, the temperature was lowered from 4500 K to

300 K in the NPT ensemble for 15 ps and the pressure was brought to 0. As a result, the carbon atoms became disordered (Fig. 2, b). The MD modeling time step was 0.5 fs, and the total time duration of the modeling was 1.035 ns.

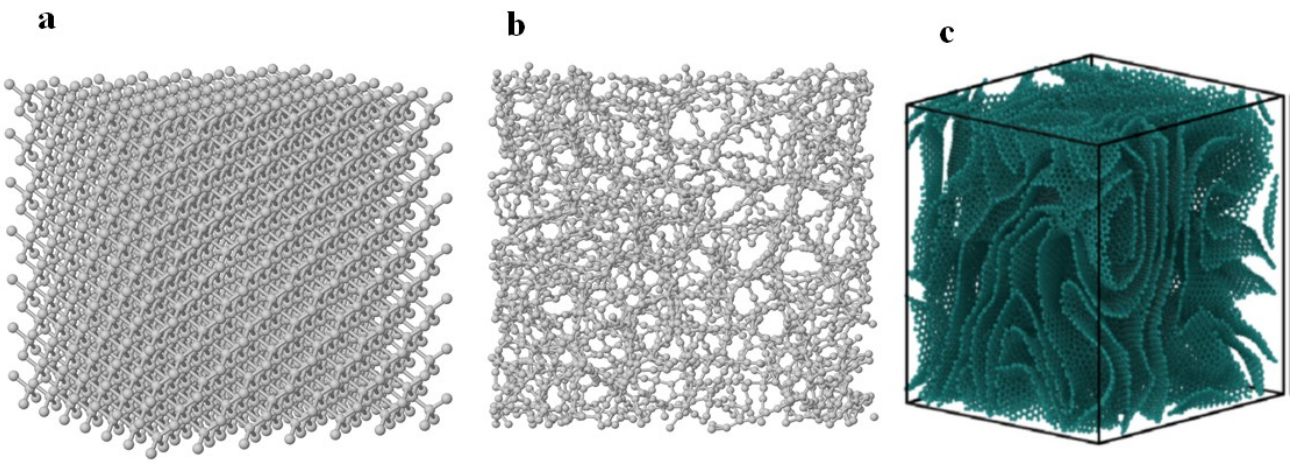


Figure 2. a) Carbon atom arrangement in step I b) End of the process in step VI c) Result copyright from Jiaqi Li[5]

In Figure 2c, Jiaqi Li and his colleagues used the EDIP potential proposed by Marx to obtain the C-C interaction potential for solid carbon. In summary, the difference between Figure 1b and c shows that the results obtained using Reaxff are flawed.

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